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Author(s): Luo, K. & Ala-Nissilä, Tapio & Ying, S. C.
Title: Polymer translocation through a nanopore: a two-dimensional Monte Carlo study
Year: 2006
Version: Final published version

Please cite the original version:

Luo, K. & Ala-Nissilä, Tapio & Ying, S. C. 2006. Polymer translocation through a nanopore: a two-dimensional Monte Carlo study. The Journal of Chemical Physics. Volume 124, Issue 3. 034714/1-5. 1089-7690 (electronic). 0021-9606 (printed). DOI: 10.1063/1.2161189.

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Polymer translocation through a nanopore: A two-dimensional Monte Carlo study

Kaifu Luo, T. Ala-Nissila, and See-Chen Ying

Citation: *The Journal of Chemical Physics* **124**, 034714 (2006); doi: 10.1063/1.2161189

View online: <http://dx.doi.org/10.1063/1.2161189>

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Polymer translocation through a nanopore: A two-dimensional Monte Carlo study

Kaifu Luo^{a)}*Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT, Finland*T. Ala-Nissila^{b)}*Laboratory of Physics Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT, Finland
and Department of Physics, Brown University, Providence, Box 1843, Rhode Island 02912-1843*See-Chen Ying^{c)}*Department of Physics, Brown University, Providence, Box 1843, Rhode Island 02912-1843*

(Received 25 October 2005; accepted 1 December 2005; published online 20 January 2006)

We investigate the problem of polymer translocation through a nanopore in the absence of an external driving force. To this end, we use the two-dimensional fluctuating bond model with single-segment Monte Carlo moves. To overcome the entropic barrier without artificial restrictions, we consider a polymer which is initially placed in the middle of the pore and study the escape time τ required for the polymer to completely exit the pore on either end. We find numerically that τ scales with the chain length N as $\tau \sim N^{1+2\nu}$, where ν is the Flory exponent. This is the same scaling as predicted for the translocation time of a polymer which passes through the nanopore in one direction only. We examine the interplay between the pore length L and the radius of gyration R_g . For $L \ll R_g$, we numerically verify that asymptotically $\tau \sim N^{1+2\nu}$. For $L \gg R_g$, we find $\tau \sim N$. In addition, we numerically find the scaling function describing crossover between short and long pores. We also show that τ has a minimum as a function of L for longer chains when the radius of gyration along the pore direction $R_{\parallel} \approx L$. Finally, we demonstrate that the stiffness of the polymer does not change the scaling behavior of translocation dynamics for single-segment dynamics.

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I. INTRODUCTION

The translocation of biopolymers through nanometer-scale pores is one of the most crucial processes in biology, such as DNA and RNA translocations across nuclear pores, protein transport through membrane channels, and virus injection.^{1–3} Moreover, translocation processes might eventually prove useful in various technological applications, such as rapid DNA sequencing,^{4,5} gene therapy, controlled drug delivery, etc.⁶ In addition to its biological relevance, the translocation dynamics is also a challenging topic in polymer physics. Accordingly, the polymer translocation has attracted a considerable number of experimental,^{7–14} theoretical,^{15–28} and numerical studies.^{29–36}

The translocation of a polymer through a nanopore faces a large entropic barrier due to the loss of a great number of available configurations. In order to overcome the barrier and to speed up the translocation, an external field or interaction is often introduced. The possible driving mechanisms include an external electric field, a chemical-potential difference, or selective adsorption on one side of the membrane. For example, in 1996, Kasianowicz *et al.*⁷ reported that an electric field can drive single-stranded DNA and RNA molecules

through the α -hemolysin channel with an inside diameter of 2 nm and that the passage of each molecule is signaled by the blockade in the channel current.

Inspired by the experiments,⁷ a number of recent theories^{15–28} have been developed for the dynamics of polymer translocation. Even without an external driving force, polymer translocation remains a challenging problem. To this end, Sung and Park¹⁶ and Muthukumar¹⁹ considered equilibrium entropy of the polymer as a function of the position of the polymer through the nanopore. The geometric restriction leads to an entropic barrier. Standard Kramer analysis of diffusion through this entropic barrier yields a scaling prediction of the translocation time $\tau_{\text{tran}} \sim N^2$ for long chains. However, as Chuang *et al.*²³ noted, this quadratic scaling behavior is at best only marginal for phantom polymers and cannot be correct for a self-avoiding polymer. The reason is that the equilibration time $\tau_{\text{equil}} \sim N^2$ for a phantom polymer and $\tau_{\text{equil}} \sim N^{1+2\nu}$ for a self-avoiding polymer, where ν is the Flory exponent [$\nu=3/4$ and $3/5$ in two-dimensional (2D) and three-dimensional (3D), respectively]. Thus the exponent for τ_{equil} is larger than two for self-avoiding polymers, implying that the translocation time is shorter than the equilibration time of a long chain, thus rendering the concept of equilibrium entropy and the ensuing entropic barrier inappropriate for the study of translocation dynamics. Chuang *et al.*²³ performed numerical simulations with Rouse dynamics for a 2D lattice model to study the translocation for both phantom and self-avoiding polymers. They decoupled the

^{a)}Author to whom correspondence should be addressed. Electronic mail: luokaifu@yahoo.com

^{b)}Electronic mail: tapio.ala-nissila@tkk.fi

^{c)}Electronic mail: ying@physics.brown.edu

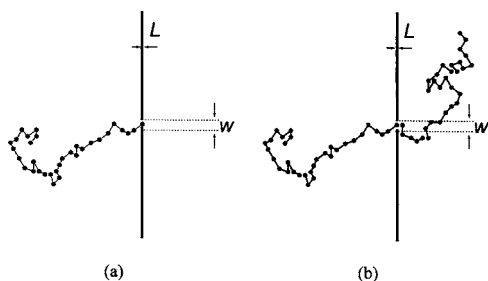


FIG. 1. (a) A polymer is initially placed on the one side of the wall with the first monomer in the pore. (b) The middle of a polymer is initially placed in the center of the pore. The length and width of the pore are L and W , respectively.

translocation dynamics from the diffusion dynamics outside the pore by imposing the artificial restriction that the first monomer, which is initially placed in the pore, is never allowed to cross back out of the pore [see Fig. 1(a)].²³ We will refer to the translocation time obtained this way as τ_{tran} . Their results show that for large N , translocation time τ_{tran} scales approximately in the same manner as equilibration time, but with a larger prefactor.

In the present work we consider a polymer which is initially placed symmetrically in the middle of the pore, as in Fig. 1(b). In this case, without any external driving force or restriction, the polymer escapes from the hole either to the left or the right side of the pore in an average time defined as the escape time τ .³⁷ It is clear that τ_{tran} and τ are different. Namely, the translocation time τ_{tran} includes events where the middle segment reaches the center of the pore but then the first segment returns to the entrance of the pore and the whole translocation process begins all over again. Numerically, τ can be sampled much more efficiently than τ_{tran} , leading to a more accurate determination of the scaling behavior. We will show numerically that $\tau \sim N^{1+2\nu}$, in the same manner as found previously for τ_{tran} . Recently, Wolterink *et al.*²⁸ have studied the translocation dynamics scaling for a 3D lattice model of a polymer. They have also found that τ scales as $\tau \sim N^{1+2\nu}$, in agreement with the present work.

In this study, we investigate the translocation dynamics in a 2D lattice model by focusing on τ . In particular, we

investigate the effect of varying the pore length on the polymer translocation. The dependence of the translocation dynamics on the stiffness of the polymer is also considered. The paper is organized as follows: In Sec. II we introduce the fluctuating bond model. In Sec. III using our approach we examine the polymer translocation through short and long pores. We obtain very accurate estimates for the scaling exponents as a function of N and find the scaling function describing crossover between short and long pores. Our results are summarized in Sec. IV.

II. THE FLUCTUATING BOND MODEL

The fluctuating bond (FB) model³⁸ combined with single-segment Monte Carlo (MC) moves has been shown to provide an efficient way to study many static and dynamic properties of polymers. Here we use the 2D lattice FB model for MC simulations of a self-avoiding polymer, where each segment excludes four nearest and next-nearest-neighbor sites on a square lattice. The bond lengths b_i are allowed to vary in the range $2 \leq b_i \leq \sqrt{13}$ in units of the lattice constant, where the upper limit prevents bonds from crossing each other. The stiffness of the chain is controlled through an angle-dependent potential^{39,40} $U/k_B T = -(J/k_B T) \sum_{j=1}^{N_{\text{FB}}-1} \times \cos(\phi)$, where J is the interaction strength, N_{FB} is the number of segments in the chain, ϕ is the angle between two adjacent bonds, k_B is the Boltzmann constant, and T is the absolute temperature. Dynamics is introduced in the model by Metropolis moves of a single segment, with a probability of acceptance $\min[e^{-\Delta U/k_B T}, 1]$, where ΔU is the energy difference between the new and old states. As to an elementary MC move, we randomly select a monomer and attempt to move it onto an adjacent lattice site (in a randomly selected direction). If the new position does not violate the excluded-volume or maximal bond-length restrictions, the move is accepted or rejected according to Metropolis criterion. N elementary moves define one MC time step.

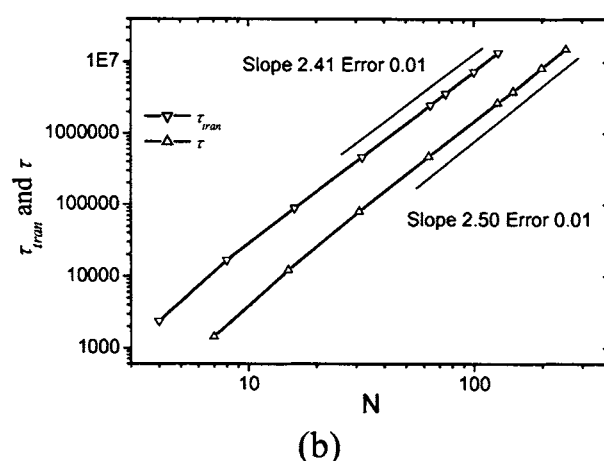
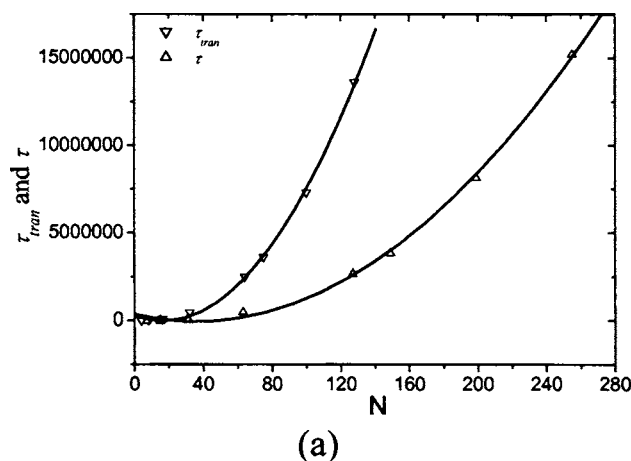


FIG. 2. (a) Average translocation time and escape time τ as a function of the chain length N . (b) A log-log plot of (a). The length and width of the pore are 3 and 2, respectively.

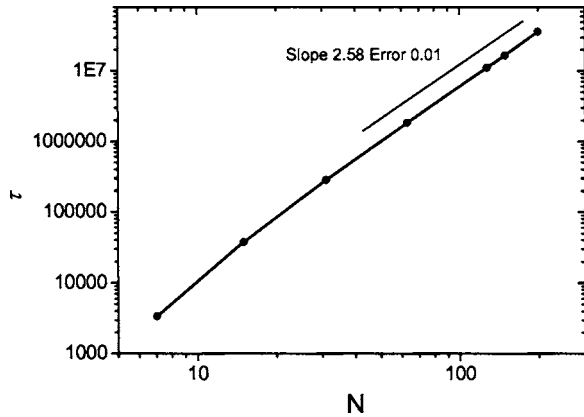


FIG. 3. Average τ as a function of the chain length of stiff polymers. The length and width of the pore are 3 and 2, respectively.

III. RESULTS AND DISCUSSION

A. Polymer translocation through a short nanopore

In this section, we present the results for the escape time τ for a lattice model of polymers. For the same model, we also studied the translocation time τ_{tran} defined by Chuang *et al.*²³ using the restriction that the first monomer cannot back out of the pore. We used the same pore size for both cases (length of $L=3$ and width of $w=2$ lattice units). Numerical studies were done for a number of different chain lengths N , with several thousand runs for each case.

In Fig. 2(a) we show the average translocation time τ_{tran} and τ as a function of the polymer length N for the case with $J=0$. The log-log plot of Fig. 2(a) is shown in Fig. 2(b). When $N > 16$, the results versus N follow scaling to a good degree of accuracy. We find that $\tau_{\text{tran}} \sim N^{2.4 \pm 0.01}$. The scaling for the escape time is $\tau \sim N^{2.50 \pm 0.01}$. The result is very close to the expected value of $1+2\nu=2.5$ and in agreement with the 3D numerical values obtained in Ref. 28.

We have also examined τ for a relatively stiff polymer, by setting $J/k_B T = 5$.⁴⁰ In Fig. 3 we show τ as a function of N . We find that $\tau \sim N^{2.58 \pm 0.01} \sim N^{1+2\nu}$, which confirms that the stiffness of the polymer does not affect the scaling behavior of τ for single-segment dynamics.

B. Polymer translocation through a long pore

Next, we consider the influence of the pore length L on τ . In the simulations, the width of the pore is chosen as $W=7$. For a successful passage through the pore of length L , the mass center of the polymer moves a distance of $L/2 + R_g$, so the time it takes can be estimated to be

$$\tau \sim \frac{(R_g + L/2)^2}{D} \sim \begin{cases} \frac{R_g^2}{D} \sim N^{1+2\nu}, & L \ll R_g \\ \frac{L^2}{D} \sim N^1, & L \gg R_g. \end{cases} \quad (1)$$

This result indicates that there is a crossover as a function of R_g/L such that for $L \ll R_g$, scaling follows the previous short pore result, while for $L \gg R_g$, the scaling behavior changes to $\tau \sim N$. Figure 4(a) shows our numerical data, where crossover is clearly seen. In Fig. 4(b) we show data for a very long pore with $L=800$, which confirms the linear scaling behavior.

In general, we can write a scaling form for τ as

$$\tau \sim \frac{R_g^2}{D} f\left(\frac{R_g}{L}\right), \quad (2)$$

where $f(x)$ is a scaling function. Using Eq. (1), we obtain

$$\tau \frac{D}{R_g^2} \sim f\left(\frac{R_g}{L}\right) \sim \begin{cases} \text{const}, & L \ll R_g \\ \frac{L^2}{R_g^2}, & L \gg R_g. \end{cases} \quad (3)$$

Using the data in Fig. 4, we plot the scaling function $f(x)$ in Figs. 5(a) and 5(b). From Fig. 5(a), we find that $f(x) \sim \text{const}$ for $L \gg R_g$, and in Fig. 5(b) we show the other limit on a log-log scale, confirming the predicted x^{-2} behavior. We note that recently Slonkina and Kdomeisky²² theoretically examined the polymer translocation through a long pore. Following the approach of Sung and Park¹⁶ and Muthukumar,¹⁹ for $L > R_g$, $\tau_{\text{tran}} \sim (L/a - N)^2$ is obtained, where a is the segment length. This result means that $\tau_{\text{tran}} \propto L^2$ for $L \gg R_g$, in contrast of our prediction here for $\tau \sim N$ in the large L limit.

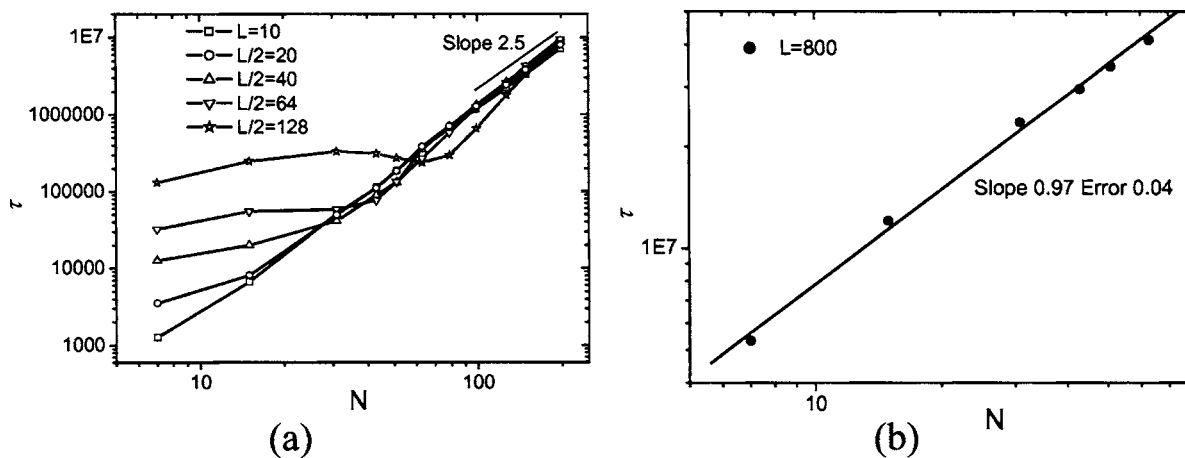


FIG. 4. (a) Average τ as a function of the chain length for polymer translocation through the long pore. (b) Average τ as a function of the polymer length for short polymer translocation through a very long pore. The pore width is 7.

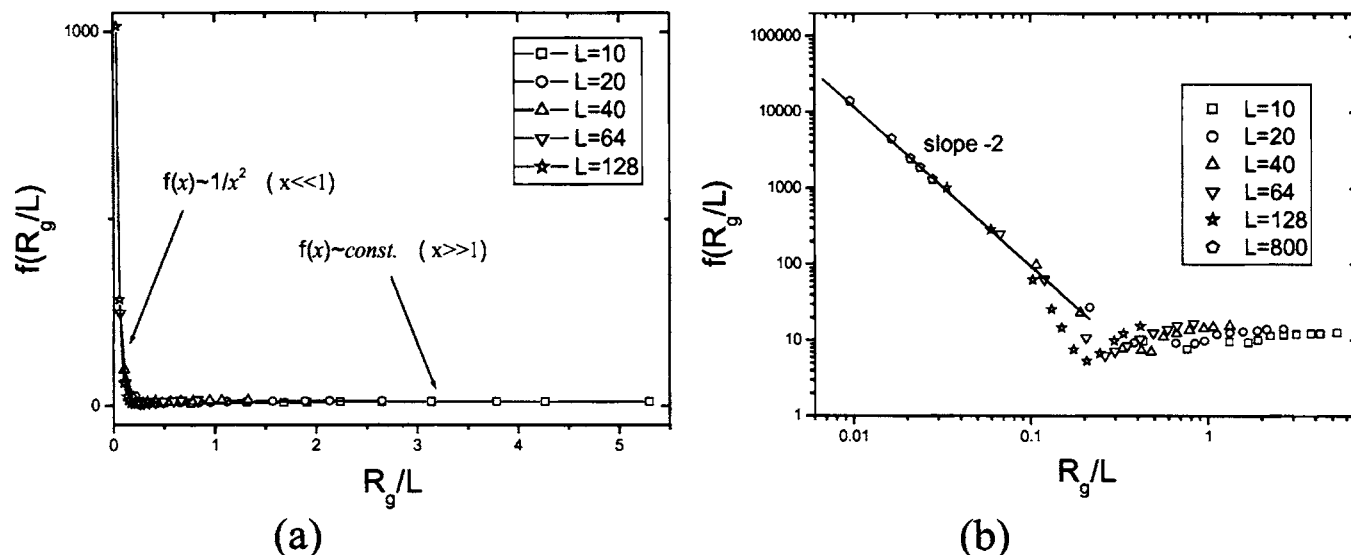


FIG. 5. (a) Scaling function for polymer escape through a long pore. (b) A log-log plot of (a).

A particularly interesting question concerns the influence of the pore length to the actual translocation dynamics with fixed N . This problem has been theoretically addressed by Muthukumar²⁰ who investigated the free-energy barrier and average translocation time for the movement of a single Gaussian chain from one sphere to another larger sphere through pores of different lengths. In Ref. 20, it was found that $\tau_{\text{tran}}(L)$ has a minimum for an “optimal” value of L_0 where translocation is fastest, and a threshold value L_c . This result was explained to be due to interplay between polymer entropy and pore-polymer interaction energy. In the first regime where $L < L_c$, $\tau_{\text{tran}}(L)$ first decreases and then increases with L , the entropic barrier mechanism dominates polymer translocation. In the other regime $L > L_c$, $\tau_{\text{tran}}(L)$ increases with L , and polymer translocation is controlled by the pore-polymer interaction. The existence of L_c thus corresponds to an apparent cancellation between the gain in translocation rate arising from the entropic part and the loss in the rate associated with the pore-polymer interaction.

In Fig. 6 we show our numerical data for a fixed chain of length $N=51$. Most strikingly, our result shows that the two regimes for the dependence of τ on the pore length are present here without any explicit pore-polymer interaction

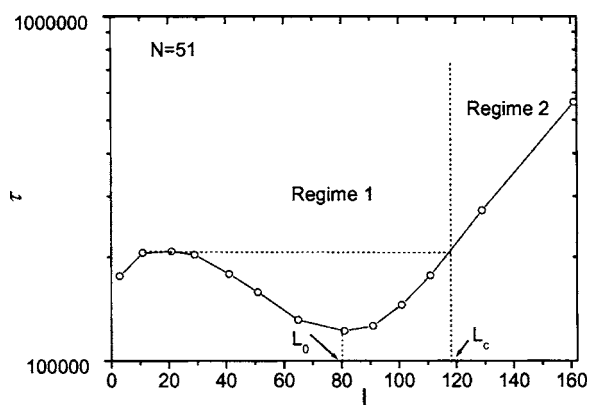


FIG. 6. (a) The effect of the pore length L on average τ for chain of length $N=51$. The pore width is 7.

potential. Thus, the existence of an optimal pore length is a generic phenomenon in polymer translocation. We find that the optimal value of L_0 , corresponds to the radius of gyration of the polymer along the pore direction, R_{\parallel} . The escape of the polymer consists of two steps. In the first step with average duration τ_1 , one end of the polymer reaches an edge of the pore. During the second step of average duration τ_2 , the other end of the polymer reaches this edge of the pore. For $L > L_0$, $\tau_1 = \tau_1(L)$ increases with L because the polymer has to move a longer distance for increasing L , and $\tau_2 = \tau_2(N)$ depends on the chain length N , but is almost independent of the pore length. Thus the total time, $\tau = \tau_1(L) + \tau_2(N)$, increases with L . For $L < L_0$, τ goes down with increasing L . Further support for the existence of an optimal pore length comes from the results of Slonkina and Kolomeisky²² for an ideal polymer where a minimum translocation time occurs at $L_0 = Na$. Our simulation results show that $L_0 \approx R_{\parallel}$, but for narrow enough pore $R_{\parallel} \approx Na$.

IV. CONCLUSION

In this paper, the polymer translocation through a nanopore in the absence of an external driving force is examined both theoretically and numerically. To overcome the entropic barrier, we consider the translocation dynamics of a polymer that is initially placed in the middle of the pore in a symmetric position, instead of using a restriction that the first monomer is never allowed to crossing back out of the pore. Our numerical results show that accurate estimates for the scaling exponents of the escape time as a function of N are obtained. Our theory predicts that the length of the pore plays a very important role in polymer translocation dynamics. For $L \ll R_g$, the escape time τ with polymer length N satisfies $\tau \sim N^{1+2\nu}$, while for $L \gg R_g$, $\tau \sim N$ is observed. We also numerically find the scaling function describing crossover between short and long pores and show that τ has a minimum as a function of L for longer chains. In addition, our numerical results show that the stiffness of a polymer does not change the scaling behavior of translocation dynamics.

ACKNOWLEDGMENT

This work has been supported in part by a Center of Excellence grant from the Academy of Finland.

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